# AN ULTRAVIOLET BASED METHYL MERCAPTAN SYSTEM FOR HALITOSIS USING AN OPTICAL FIBRE SENSOR

SUZALINA BINTI KAMARUDDIN

MASTER OF SCIENCE

UNIVERSITI MALAYSIA PAHANG

## SUPERVISOR'S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Master of Science.

_____

(Supervisor's Signature)

Full Name : PROFESOR MADYA TS. DR. HADI BIN MANAP

Position : SENIOR LECTURER

Date : 20 FEBRUARY 2020

## STUDENT'S DECLARATION

I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

_____

(Student's Signature)

Full Name : SUZALINA BINTI KAMARUDDIN

ID Number : MKE 13001

Date : 20 FEBRUARY 2020

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SUZALINA BINTI KAMARUDDIN

Thesis submitted in fulfillment of the requirements
for the award of the degree of
Master of Science

Faculty of Electrical and Electronic Engineering Technology

UNIVERSITI MALAYSIA PAHANG

FEBRUARY 2020

## ACKNOWLEDGEMENTS

Alhamdulillah, I thank Allah for the years of ups and downs of this Masters study. This beautiful journey will always be the foundation of the great destination. I would like to express sincere gratitude to those who have provided all the supports and encouragement for me to finally finish my study. First and foremost, I would like to thank my supervisor, Prof. Madya TS. Dr. Hadi Manap, for his guidance and assistance throughout my study. His great enthusiasm, insightful perspective and work ethics have helped me grow professionally and extensively. His continuous understanding and kind words are the inspiration that keep me going on the right path.

My sincere gratitude goes to the Faculty of Engineering Technology (FTEK) at Universiti Malaysia Pahang for supporting my work with the allocated education grant and usage of facilities. The generous deal allowed me to carry out my experiment smoothly and getting the best out of it.

I would also like to express my sincere gratitude to the management of Malaysian Meteorological Department (MMD) for giving me the chance to further my study while I am working as the Meteorological Officer.

My biggest thank and never ending loves to my late father who initiated the strong will to further my study and to my mother who always believe in whatever I do.

Last but not least, I thank my husband, Muhammad Ridzaudin, for his unconditional support, love, understanding, encouragement, assistance and patience while I was completing my study. His continuing willingness to care for our children to lessen my burden and help me go through the milestones of the thesis writing is deeply appreciated. To all my six children, you are my strength and my reason to live.

# ABSTRAK

Halitosis adalah bau busuk dari mulut, yang berasal terutamanya dari pereputan bakteria yang menghasilkan sebatian sulfur tidak seimbang (VSC) terutamanya methyl mercaptan ($CH_3SH$). Ia adalah masalah kritikal yang telah menjadi kebimbangan masyarakat dan memerlukan prosedur yang teratur untuk pengesanan. Kebanyakan sistem atau kaedah pengesanan semasa gagal mengenal pasti dan membezakan VSC, sensitif terhadap persekitaran dan memberikan hasil yang tidak dapat diukur. Didapati bahawa sistem pengesanan optik adalah lebih sesuai digunakan berbanding *gas chromatograph*, *portable sulphide monitors*, *electronic noses* dan ujian kimia atau enzim. Tujuan utama tesis ini adalah untuk membina alat pengesan halitosis berasaskan sinar lampau ungu (UV) dan sensor kabel optik (OFS). Alat ini diguna untuk mendapatkan spektra keratan rentas penyerapan bagi $CH_3SH$, komponen utama VSC untuk analisis dan mencari rantau panjang gelombang sistem. Untuk tujuan validasi sistem, penilaian terhadap kemungkinan gangguan daripada gas-gas pernafasan dan pengiraan kepekatan $CH_3SH$ dilakukan. Metodologi penyelidikan berasaskan kaedah spektroskopi penyerapan. Prinsip kerja sistem ini melibatkan pergerakan cahaya UV dari sumbernya melalui kabel fiber dan kemudian dimodulasi oleh bahan di dalam zon modulasi sebelum dikesan oleh spektrometer yang juga dihubungkan dengan kabel fiber. Teknik laluan terbuka berlaku di dalam zon modulasi. Dengan menggunakan sistem pengesanan ini, jenis gas boleh dikenalpasti melalui ciri unik yang ada pada setiap gas. Menggunakan persamaan daripada Hukum *Beer Lambert* yang diubahsuai, keratan rentas penyerapan, $\sigma$ bagi $CH_3SH$ diperolehi daripada eksperimen yang dibuat menggunakan gas $CH_3SH$ sebagai bahan ujikaji, dan graf berkaitan diplot. Keputusan yang didapati mempunyai korelasi yang tinggi (*coefficient* = 0.99) dengan data teori yang didapati daripada pangkalan data *UV-VIS MPI Mainz*. $\sigma$ bagi oksigen ($O_2$) dan karbon dioksida ($CO_2$) diperolehi untuk tujuan validisasi. Penilaian gas $CH_3SH$ dengan gas pernafasan, air ($H_2O$), $O_2$ dan $CO_2$ mendapati bahawa tiada isu gangguan oleh gas pernafasan bagi rantau panjang gelombang 200 hingga 270 nm. Dan, kepekatan gas $CH_3SH$ memberi nilai 97.46 ppm iaitu menghampiri 100 ppm seperti yang dinyatakan oleh pengeluar. Akhirnya, sistem pengesan yang dicadangkan ini berupaya mengesan gas $CH_3SH$ dalam rantau UV-C, dengan rantau panjang gelombang 200 hingga 210 nm adalah pilihan terbaik untuk sistem pengesanan berasaskan UV, dimana puncak penyerapan berada di sini. Sistem ini adalah sesuai dan boleh diharapkan sebagai pengesan halitosis. Sistem pengesanan berasaskan UV dengan gabungan OFS dibina daripada komponen yang sedia ada di pasaran dapat digunakan untuk mengesan halitosis, kenalpasti gas yang berbeza, tidak sensitif terhadap gangguan gas lain dan boleh diukur untuk penggunaan rutin klinik dalam bidang pergigian.

## ABSTRACT

Halitosis is a foul smells from the mouth, mainly originate from the putrefactive bacteria that produce volatile sulphur compounds (VSCs), predominantly methyl mercaptan ($CH_3SH$). It has become public concerned which needs well structured procedure for detection purpose. However, current systems or methods failed to identify and distinguish main components of VSCs, sensitive to the environment and provide immeasurable results. Optical detection system is found to be more reliable than gas chromatograph, portable sulphide monitors, electronic noses and chemical or enzymatic tests. Main purpose of this study is to develop an ultraviolet (UV) based methyl mercaptan system using optical fibre sensor (OFS) to detect halitosis. The proposed system is utilised to obtain the absorption cross section spectra of $CH_3SH$, the main component of VSCs for the analyses and wavelength spectral determination. To validate the proposed system, cross sensitivity evaluation with breathing gases and calculation of $CH_3SH$ gas concentration is performed. Methodology of the study is based on the absorption spectroscopy method. The working principle of the proposed system involved propagation of UV light signal from its source through the input fibre and then modulated by measurand in the modulation zone before it is sensed by spectrometer as the detector through the output fibre. The modulation zone is where the open path technique will take place. Each gases has their unique characteristic which corresponds to their identification and can be determined using this detection system as the measurand. By manipulating the Beer Lambert Law equation, the datasets of absorption cross section, $\sigma$ for $CH_3SH$ was obtained and plotted against wavelength. The result was found to be highly correlated (coefficient = 0.99) with theoretical datasets from the MPI Mainz UV-VIS database. $\sigma$ for $O_2$ and $CO_2$ were obtained for system validation purposes. Cross sensitivity evaluation of $CH_3SH$ which was carried out with breathing gases $O_2$, $CO_2$ and water ($H_2O$) proved that interference was not an issue for UV wavelength region of 200 to 270 nm. And, the calculated $CH_3SH$ gas concentration is 97.46 ppm almost reach the 100 ppm that was stated by manufacturer. Finally, the proposed system is capable of detecting $CH_3SH$ in the UV-C region, with the best potential band of 200 to 210 nm where the excellent peak located. The UV based detection system with OFS which was constructed with available manufactured components is able to detect halitosis, distinguished different gases, not sensitive to interference and can produce measurable results for routine clinical usage in the dental field.

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| | |
|---|---|
| $T$ | Absolute Temperature |
| $A$ | Absorbance |
| $\sigma$ | Absorption Cross Section |
| $N_A$ | Avogadro's Constant |
| $\rho$ | Gas Density |
| $N$ | Gas Concentration |
| $R$ | Ideal Gas Constant |
| $I_o$ | Incident Intensity |
| $n$ | Mass of Substance |
| $\omega$ | Molecular Weight |
| $l$ | Path Length |
| $P$ | Pressure |
| $t$ | Transmittance |
| $I$ | Transmitted intensity |
| $V$ | Volume |
| $\lambda$ | Wavelength |

## LIST OF ABBREVIATIONS

| | |
|---|---|
| BANA | Benzoyl-DL-arginine-naphthylamide |
| BC | Before Century |
| CCD | Charge Couple Device |
| $CH_3SH$ | Methyl Mercaptan |
| $CH_3CH_3SH$ | Dimethyl Sulphide |
| $CO_2$ | Carbon Dioxide |
| FPD | Flame Photometric Detector |
| GC | Gas Chromatography |
| $H_2S$ | Hydrogen Sulphide |
| $H_2O$ | Water Vapour |
| MAO-A | Monoamine Oxidase Type-A |
| MEMs | Micro-Electromechanical Systems |
| MS | Mass Spectrometer |
| $N_2$ | Nitrogen |
| $O_2$ | Oxygen |
| OFS | Optical Fibre Sensor |
| OT | Organoleptic testing |
| POF | Plastic Optical Fibre |
| UV | Ultraviolet |
| VSC | Volatile Sulphur Compound |

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